Glass and Ceramics, Vol. 71, Nos. 1 – 2, May, 2014 (Russian Original, Nos. 1 – 2, January – February, 2014)

UDC 666.1.519.713:539.216

MODELING OF THE ELASTIC ELECTRONIC POLARIZATION OF HIGH-TEMPERATURE GLASS

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Translated from *Steklo i Keramika*, No. 2, pp. 7 – 9, February, 2014.

An efficient mathematical model of the elastic polarization of a material in the condensed state is examined. The results of computer modeling of the optical spectra of four raw-material crystalline oxides as well as the spectral properties based on them are presented for three different samples of refractory glasses.

Key words: permittivity, index of refraction, composite material, computational experiment.

Advances in the most diverse fields of science and technology often involve the use of special oxide glasses which must be electrically conducting and resist oxidation by the atmosphere at temperatures to 2000°C. Such highly uniform and corrosion-resistant refractory materials are needed to intensify pyrometallurgical processes and increase the quality of smelted alloyed steels and alloys and chemical synthesis of solid electrolytes used in chemical sources of electricity and so forth.

High-temperature glass with a complex composition is characterized by a complex of valuable operating qualities: a combination of quite high values of the refractive index, mechanical characteristics and strain temperature; relatively low values of the linear thermal expansion coefficient; and, extraordinary resistance to alkali. These particularities make such glasses promising optical materials capable of operating at high temperatures in chemically aggressive media. In addition, high-temperature glass has been attracting attention recently in connection with its possible application as a laser material.

The results of an investigation of the physical and mechanical properties of four types of refractory glass in the system Al_2O_3–SiO_2–R_2O_3 (R corresponds to Sc, Y, La or Er), synthesized by direct high-frequency melting in a cold crucible are presented in [1]. Physical measurements were conducted on blocks up to 1.6 kg in size with no inclusions or unreacted components. An analysis performed by the present authors showed that the values of the index of refraction, physical density, Young's modulus, shear modulus and Poisson ratio of the samples studied are all much greater than the analogous values characteristic for ordinary quartz glass.

In turn, in the conventional procedure, which is complex and characterized by large expenditures of different kinds of resources, the component composition of commercial glass samples with the desired properties is sought in multiple steps. The extant situation can be radically changed by adopting in the technological processes analytical methods oriented toward computer modeling of the synthesized properties of materials.

Thus, the aim of the research described above was to construct an efficient mathematical model of the elastic electronic polarization of the materials of interest, making it possible to calculate in practice their theoretical optical spectra which are as close as possible to the actual data obtained in real physical measurements.

It is assumed within the framework of the quantum theory that the planetary model of the atom, first proposed at the beginning of the last century, can be explain wholly and completely some features of the electronic spectra of material particles whose shells contain more than one electron. For this reason the model is supplemented by the hypothesis that the electronic orbits are present in an atom are elliptical rather than circular. However, in spite of being theoretically well-grounded modern quantum-mechanical calculations remain too imperfect and require too much time to perform modern applied calculations [2, 3].

On the other hand the fundamental research performed during the last decade at the juncture of the classical theories of polarization of dielectrics and automatic control show quite objectively that the electronic configurations of complex materials can be adequately represented by corresponding sets of atomic orbitals populated by paired electrons moving only on circular orbits. The complete set of the processes analyzed is effectively described by systems of linear equations of damped harmonic oscillations formed taking ac-

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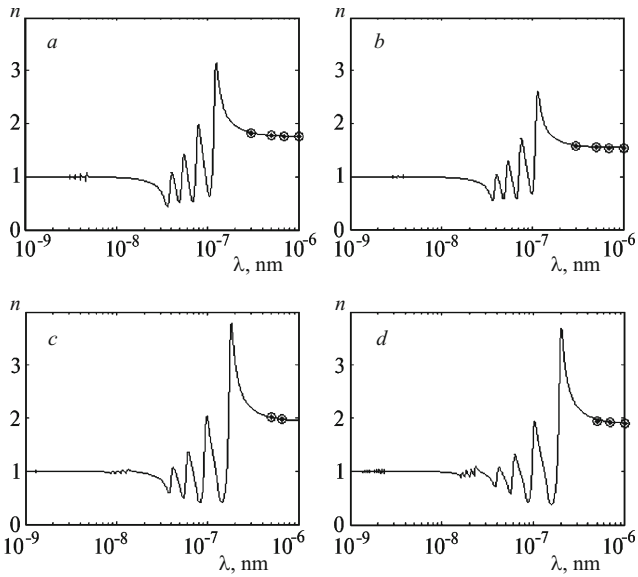

Fig. 1. Electron-optical spectra of raw material components of glass: *a*) crystalline Al_2O_3; *b*) crystalline SiO_2; *c*) crystalline Sc_2O_3; *d*) crystalline Y_2O_3; solid lines) computed data; points) data from experimental measurements.

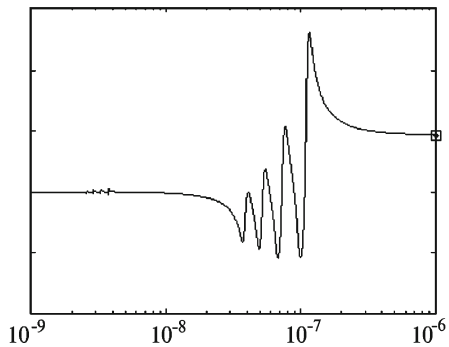

Fig. 2. Electron-optical spectrum of quartz glass (SiO_2 — 100%).

count of all types of electronic pairs occurring in the electronic configurations of the constituent particles of the experimental samples, and the equation of the complex permittivity based on them can be expressed in the form of its original 'cybernetic model' [4 – 6].

Since the control data on the physical measurements of the optical refractive index $n(\lambda)$ of different substances at long wavelengths [7] as required for an effective cybernetic model of the electronic polarization do exist, a series of computational experiments was conducted initially for computer modeling of the optical spectra of crystalline aluminum, silicon, scandium and yttrium oxides.

Plots of $n(\lambda)$ for the raw material components of high-temperature glass which were obtained by a computational method [5, 8, 9] based on reference data [10] are displayed in Fig. 1.

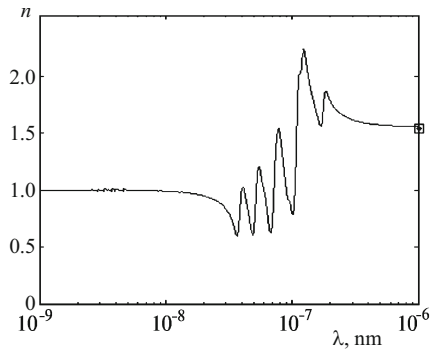

Fig. 3. Electron-optical spectrum of the glass Al_2O_3:SiO_2:Sc_2O_3 = 30:60:10 wt.%.

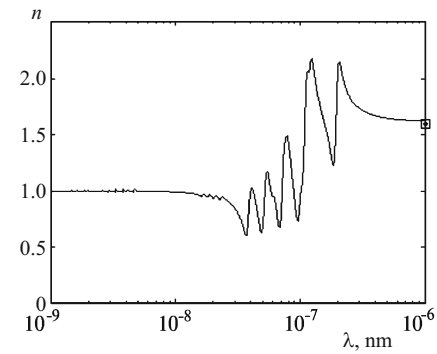

Fig. 4. Electron-optical spectrum of the glass Al_2O_3:SiO_2:Y_2O_3 = 20:50:30 wt.%.

Analysis of the simulation characteristics presented shows that the computational method makes it possible to effectively model the optical properties of the oxide crystals under study. Indeed, all continuous simulation characteristics $n(\lambda)$ obtained on the basis of a fundamental theoretical calculation correspond well both quantitatively (agreement with control points) and qualitatively (overall replication of the curve fitting the control data) to the point array.

It is well known that any ceramic samples, high-temperature glasses being one form, always comprise a multicomponent system formed by integration of the crystalline, glassy and gas phases of matter. In turn, electronic polarization is an additive property of any material that does not depend on its structure or the aggregate state of the material. Therefore, optimized models of the elastic electronic polarization obtained for the crystalline phases of the raw material oxides studied should also be effective in modeling the optical properties of the same substances in the glass phase.

The results of computer modeling of the long-wavelength dependence of the optical refractive index for high-temperature glasses with the oxide content of oxides 100 wt.% SiO_2, Al_2O_3:SiO_2:Sc_2O_3 = 30:60:10 wt.% and Al_2O_3:SiO_2:Y_2O_3 = 20:50:30 wt.% are displayed in Figs. 2 – 4 (solid lines correspond to the computed spectra, points depict data from physical measurements).

Analysis of the simulation characteristics shows that the computed optical spectra $n(\lambda)$ of the samples studied are practically equivalent to their actually observed values.

Therefore, the computational methodology described here is very effective and versatile for modeling the optical properties of crystalline oxides and their glass-forming melts.

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